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MODTRAN:
A MODERATE RESOLUTION MODEL FOR LOWTRAN 7

Alexander Berk,
Lawrence S. Bernstein, and David C. Robertson
Spectral Sciences, Inc.
99 South Bedford Street, #7
Burlington, MA 01803

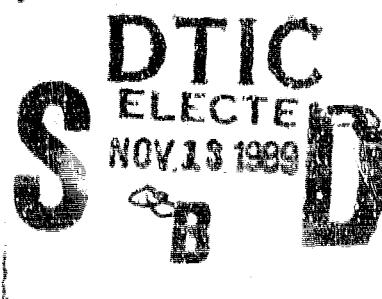
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"This technical report has been reviewed and is approved for publication"



LEONARD W. ABREU
Contract Manager
Atmospheric Effects Branch
Optical/Infrared Technology Division



ROBERT R. O'NEIL, Chief
Atmospheric Effects Branch
Optical/Infrared Technology Division

FOR THE COMMANDER



R. EARL GOOD, Director
Optical/Infrared Technology Division

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approximation is used to reduce paths through the atmosphere to an equivalent single-layer path.

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1. INTRODUCTION

The LOWTRAN computer codes, with LOWTRAN 7⁽¹⁾ being the most current version, are widely used to calculate atmospheric transmittance and/or radiance in the infrared, visible and near ultraviolet spectral regions; LOWTRAN 7 has been extended to include the microwave spectral region. The code is easily used, runs quickly and provides the user with a wide variety of atmospheric models and options. Its spectral resolution is 20 cm^{-1} Full Width/Maximum (FWHM) with calculations being done in 5 cm^{-1} increments.

This final technical report describes work done to increase LOWTRAN's spectral resolution from 20 to 2 cm^{-1} (FWHM). Specifically, the technical objectives for this program were:

- to develop algorithms providing 2 cm^{-1} resolution (FWHM);
- to model molecular absorption of atmospheric molecules as a function of temperature and pressure;
- to calculate band model parameters for twelve LOWTRAN molecular species; and
- to integrate the LOWTRAN 7 capabilities into the new algorithms, maintaining compatibility with the multiple scattering option.

MODTRAN, the final product of this effort, is a moderate resolution LOWTRAN code. Molecular absorption is calculated in 1 cm^{-1} spectral bins, while the other parts of the calculation remain unchanged. The molecular species affected are:

water vapor, carbon dioxide, ozone, nitrous oxide, carbon monoxide, methane, oxygen, nitric oxide, sulfur dioxide, nitrogen dioxide, ammonia and nitric acid.

Their absorption properties (the band model parameters) are calculated from the HITRAN line atlas,⁽²⁾ which contains all lines in the $0 - 17,900\text{ cm}^{-1}$

spectral region that have significant absorption for atmospheric paths. The increased resolution of MODTRAN spans the same spectral region; calculations at larger wavenumbers, the visible and ultraviolet spectral regions, are performed at the lower spectral resolution, 2 cm^{-1} .

Creation of this new code, MODTRAN, required the development and integration of a completely new set of band models for calculating transmittance. The increased spectral resolution is achieved using an approach developed in a previous effort which resulted in a 5 cm^{-1} option^(3,4) to LOWTRAN 5.⁽⁵⁾ In this approach, band model parameters were calculated from the HITRAN database and used to determine the equivalent width of the absorbing molecular gases in 5 cm^{-1} spectral intervals. In the present work, the band model parameters are calculated in 1 cm^{-1} intervals. The molecular transmittance calculation for each bin has three elements. First, the Voigt lineshape of an "average" line is integrated over the 1 cm^{-1} interval; when a bin contains more than one line of a given species, the lines are assumed to be randomly distributed with statistical overlap; finally, the contribution from lines whose centers are in nearby bins is calculated as a molecular "continuum" component. The other LOWTRAN components, which have insignificant spectral structure at 1 cm^{-1} , are calculated at their 5 cm^{-1} increments and interpolated to arrive at the total transmittance for each interval. The calculational grid consists of non-overlapping 1 cm^{-1} bins, which are degraded to the desired spectral resolution with an internal triangular slit function. Since these bins are square and non-overlapping, the nominal spectral resolution of MODTRAN is reported as 2 cm^{-1} (FWHM).

The new MODTRAN subroutines are written in portable ANSI standard FORTRAN and constructed so that their interfacing with LOWTRAN 7 minimizes coding changes. These additional elements do not interfere with the regular operation of LOWTRAN 7; rather they represent an additional capability for higher spectral resolution. All the usual LOWTRAN options like aerosol models, path options, multiple scattering model, user-specified profiles, etc., have been maintained. The large amount of molecular data required for the increased spectral resolution has necessitated using an external data file or band model tape.

The comparison of MODTRAN and LOWTRAN 7 calculations shown in Figure 1 illustrates the increased spectral resolution. The figure shows the transmittance calculated at 2 and 20 cm^{-1} resolution for a low altitude slant path through the US Standard Atmosphere. The 2 cm^{-1} curve results from the internal triangular slit function (IFWHM=2), and the 20 cm^{-1} curve is the regular LOWTRAN 7 result calculated in 5 cm^{-1} steps. The MODTRAN calculation resolves line structure below 2180 cm^{-1} (primarily water), the band center of the N_2O fundamental at 2220 cm^{-1} , and the C^{13}O_2 band center at 2284 cm^{-1} .

An overview of MODTRAN is presented in Section 2. In the subsequent two sections, calculation of the band model parameters and the transmittance formulation are described. The changes to LOWTRAN 7 and the new MODTRAN subroutines are described in Section 5. In Section 6, illustrative MODTRAN calculations for initial validation are discussed.

Conclusions are discussed in the final section.

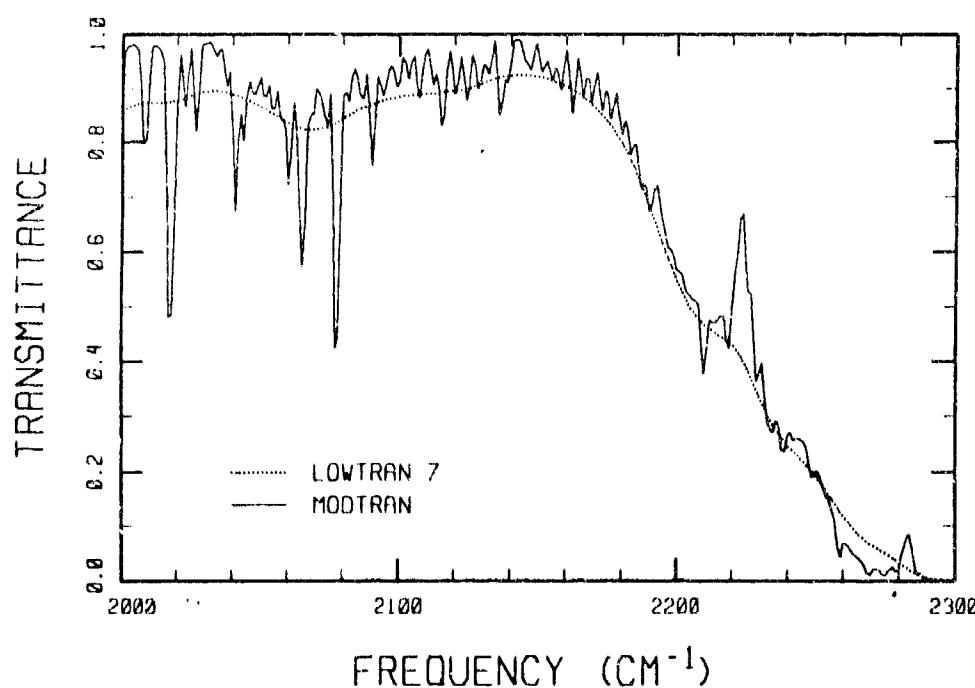


Figure 1. Atmospheric Transmittance for a Slant Path from 5 to 10 km at 15° from Zenith and Through the US Standard Atmosphere with No Haze. The Solid Curve was Calculated with MODTRAN at 2 cm^{-1} Spectral Resolution, and the Dotted Curve with the Regular LOWTRAN 7 at 20 cm^{-1} Resolution.

2. THE MODTRAN CODE - AN OVERVIEW

MODTRAN is a version of LOWTRAN 7 with six additional subroutines that provide the increased spectral resolution. The input data sequence for MODTRAN is identical to LOWTRAN 7's except for two modifications, an additional parameter on Cards 1 and 4. A logical parameter, MODTRN, has been added to the front end of CARD 1

```
READ(IRD,'(I1,I4,12I5,F8.3,F7.2)')MODTRN,MODEL,ITYPE,ITEMSCT,  
1 IMULR,M1,M2,M3,M4,M5,M6,MDEF,IM,NOPRT,TBOUND,SALB ,
```

and the input to CARD 4 has been changed to integer format with a resolution parameter, IFWHM, added

```
READ(IRD,'(4I10)')IV1,IV2,IVD,IFWHM .
```

MODTRN is simply a switch which when set to F (false) causes the regular LOWTRAN 7 to be run and when set to T (true) activates MODTRAN. The parameter IFWHM, which is only read if MODTRN is true, specifies the full width at half maximum, FWHM, of an internal triangular slit function.

MODTRAN and LOWTRAN 7 differ in their approaches to calculating molecular transmittance. For several different spectral intervals LOWTRAN 7 uses a one-parameter band model (absorption coefficient) plus molecular density scaling functions. The MODTRAN band model uses three temperature-dependent parameters, an absorption coefficient, a line density parameter and an average linewidth. The spectral region is partitioned into 1 cm^{-1} bins for each molecule. Within each bin, contributions from transitions whose line centers fall within the bin are modeled separately from nearby lines centered outside of that bin, Figure 2. The absorption due to lines within the bin is calculated by integrating over a Voigt line shape.⁽⁶⁾ The Curtis-Godson^(7,8) approximation, which is accurate for the moderate temperature variations found in the earth's atmosphere, is used to replace multilayered paths by an equivalent homogeneous one.

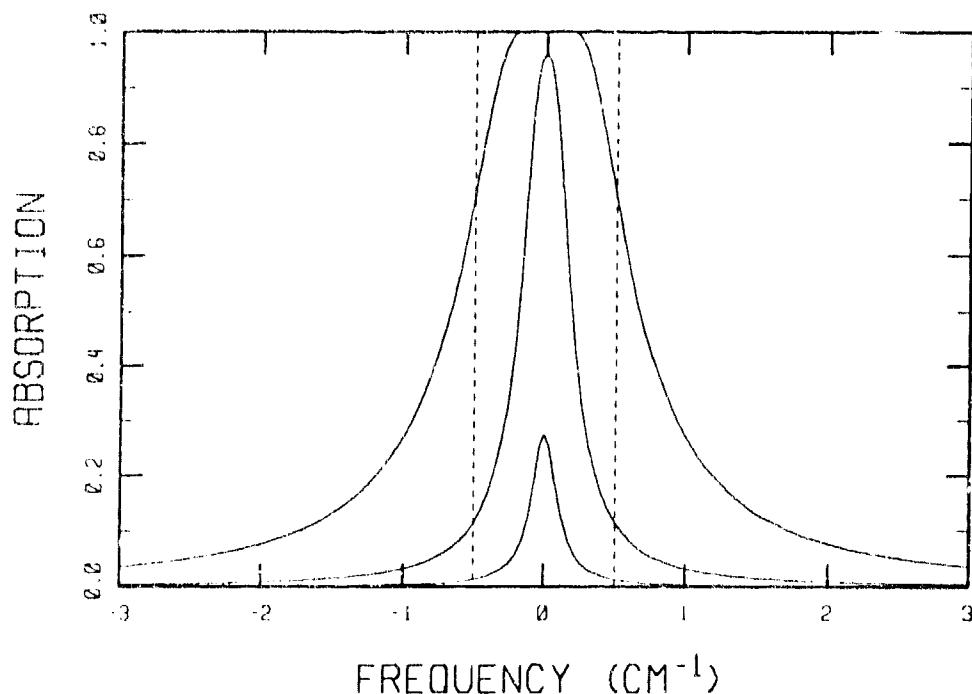


Figure 2. Absorption from Lorentzian Lines with Optical Depths of 0.1, 1, and 10. Halfwidth was set to 0.1 cm^{-1} . In the Band Model Transmittance Formulation, Absorption from Line Centers (Segment of Curves Falling Within the Spectral Bin Denoted by the Dashed Lines) is Modeled Separately from Absorption Due to Line Tails (Outside the Dashed Lines).

The k -distribution method, which is used in LOWTRAN 7's multiple scattering treatment to correct for averaging over large spectral intervals, is not used in the MODTRAN version. Because three (monochromatic) k values are used for the 5 cm^{-1} steps of LOWTRAN 7, the 1 cm^{-1} MODTRAN steps provide an equivalent accuracy for the multiple scattering option.

MODTRAN is better suited than LOWTRAN for atmospheric paths which lie completely above 30 km. This is due to the integration over the Voigt lineshape combined with the explicit temperature and pressure dependencies of the band model parameters. The Voigt lineshape is necessary at these altitudes because the Doppler linewidth is greater than the Lorentz. The 20 cm^{-1} versions of LOWTRAN suffer because they use a single set of band model parameters (nominally sea level at 296 K) coupled with spectrally

independent scaling functions for the molecular densities. It is also worth mentioning that, for paths which lie completely above 60 km, another problem arises: many of the molecules are no longer in local thermodynamic equilibrium (LTE). This means that the strengths of some molecular bands can no longer be determined from the ambient temperature. MODTRAN gives reasonable results for those bands which are in LTE; the problem is identifying those spectral regions which are not LTE. For additional information and discussion, the user is directed to the Geophysics Handbook. (9)

3. MOLECULAR BAND MODEL PARAMETERS

The basic idea behind band model techniques^(6,10,11) is to determine a set of parameters from which transmittance over finite frequency intervals can be calculated. In MODTRAN, three band model parameters are used, an absorption coefficient, a line density and a line width. The absorption coefficient measures the total strength of lines in an interval. The line density is a line strength weighted average for the number of lines in the interval, and the line width parameter is a line-strength weighted average line width.

MODTRAN uses a bin width of one wavenumber, $\Delta\nu = 1 \text{ cm}^{-1}$. Line data from the HITRAN database,⁽²⁾ the AFGL line atlas, is used to calculate the band model parameters. The tape contains data on molecular lines in the frequency range 0 to 17900 cm^{-1} . For each molecule with lines whose centers fall within a given spectral bin, the temperature dependent absorption coefficients and line densities along with the line width parameter are stored for subsequent use in calculating molecular absorption; a single temperature-dependent absorption coefficient parameter is used to determine the tail contributions to each spectral bin from lines centered in nearby bins.

In the next two subsections, the calculation of the molecular band model parameters is described, and the formatting of the data file is discussed in the third subsection. Formulas used to calculate the parameters are given, along with a discussion of their dependence on temperature and pressure.

3.1 Line Center Parameters

Each frequency bin corresponds to a 1 cm^{-1} interval and contains parameters for molecules with lines in that interval. The molecules for which band model parameters have been determined are:

H_2O , CO_2 , O_3 , N_2O , CO , CH_4 , O_2 , NO , SO_2 , NO_2 , NH_3 & HNO_3

The molecular absorption coefficients (S/d) ($\text{cm}^{-1} \text{ amagats}^{-1}$) are calculated at 5 reference temperatures:

$$T = 200, 225, 250, 275 \text{ & } 300 \text{ K} \quad . \quad (1)$$

Linear interpolation is used to calculate absorption coefficients at temperatures between 200 and 300 K. For temperatures below 200 and above 300 K, the extreme values, $(S/d)(T=200\text{K})$ and $(S/d)(T=300\text{K})$, respectively, are used. The absorption band model parameters are calculated from the individual line strengths,

$$(S/d) = \frac{1}{\Delta\nu} \sum_j S_j(T) \quad . \quad (2)$$

Here $S_j(T)$ is the integrated line strength at temperature T of the j 'th line of molecule m in bin i . The line strength at an arbitrary temperature is scaled from the HITRAN line strength at its standard temperature, $T_s = 296 \text{ K}$, by

$$S_j(T) = \frac{Q_r(T_s)Q_v(T_s)}{Q_r(T)Q_v(T)} \cdot \frac{1 - \exp(-hcv_j/kT)}{1 - \exp(-hcv_j/kT_s)} \cdot \exp\left(\frac{E_j}{k} \frac{T-T_s}{T_s}\right) S_j(T_s) \quad , \quad (3)$$

where Q_r and Q_v are the rotational and vibrational partition functions, E_j is the energy of the lower transition state, and v_j is the transition frequency. The constants are the speed of light (c), the Boltzman constant (k), and the Planck constant (h).

A collision broadened or Lorentz line width parameter γ_c^0 is defined at STP ($T_0 = 273.15 \text{ K}$, $P_0 = 1013.25 \text{ mbar}$). A single value can be stored because the pressure and temperature dependence of the Lorentz line width is easily modeled,

$$\gamma_c(T, P) = \gamma_c^0 \frac{P}{P_0} (T_0/T)^x \quad (4)$$

where the exponent x has been set to 1/2 for all molecules except CO_2 , for which $x = 3/4$. The γ_c^0 band model parameter is calculated as a line strength weighted average over the tabulated Lorentz line widths $\gamma_{c,j}(T_s)$

$$\gamma_c^0 = (T_s/T_o)^x \left[\sum_j \gamma_{c,j}(T_s) S_j(T_s) \right] / \left[\sum_j S_j(T_s) \right] . \quad (5)$$

Like the absorption coefficients, the line density band model parameters $(1/d)$ (cm) are calculated at the five reference temperatures and interpolated when used by the band model subroutines. The line density is defined by

$$(1/d) = \frac{1}{\Delta\nu} \left(\sum_{j=1}^N S_j \right)^2 / \sum_{j=1}^N S_j^2 . \quad (6)$$

This definition for the line spacing, which is derived in the appendix, produces a smaller value than the usual definition involving a sum over the square root of the line strengths.^(10,11) The new form results when account is taken of finite bin widths. The absorption of a line within a finite bin is less than its total line strength: this is consistent with a decreased value for $(1/d)$.

3.2 Line Tail Parameters

The line tail parameters consist of line contributions from lines located outside of a given bin but within $\pm 25 \text{ cm}^{-1}$. The line tail absorption coefficient band model parameters C ($\text{cm}^{-1} \text{ amagat}^{-1}$) are determined by integrating the Lorentz line shape over this interval

$$C = \frac{1}{\pi\Delta\nu} \sum_{k=i-25}^{i+25} (1-\delta_{ki}) \left\{ \frac{[(S/d) \gamma_c]_k}{(k-i)^2 + 1/4} f[(k-i)\Delta\nu] + \frac{[(S/d) \gamma_c]_k}{(k+i)^2 + 1/4} f[(k+i)\Delta\nu] \right\} , \quad (7)$$

where the delta function serves to exclude the $k=i$ term from the sum (i.e., the line center contribution), and $f[\Delta\nu]$ is a lineshape form factor. The form factor is 1.0 within 25 cm^{-1} of the line centers. Except for H_2O and CO_2 , tail contributions beyond 25 cm^{-1} are assumed negligible and not included. The usual LOWTRAN 7 water continuum consists of tail contributions from lines located beyond 25 cm^{-1} plus extrapolated (flat) values of this contribution within 25 cm^{-1} (for smoothness). For CO_2 , the continuum from FASCOD2^(12,13) has been added to the C to account for the tail contributions from lines beyond 25 cm^{-1} ,

$$C \rightarrow C + \nu_i \tanh\left(\frac{h\nu_i}{2kT}\right) \frac{T_s}{T} \tilde{C}(\nu_i) \quad . \quad (8)$$

Here, $\tilde{C}(\nu_i)$ is the frequency interpolated value from FASCOD2's block data /FCO2/. For both H_2O and CO_2 , the value of C has also been reduced by an amount equal to its value at 25 cm^{-1} from the line center since this contribution is included already in the continuum data.⁽¹⁴⁾ The C is proportional to pressure (which arises from the Lorentz line width, Equation (4))

$$C(P) = \frac{P}{P_0} C(P_0) \quad (9)$$

3.3 Parameter Data File

Because of the large amount of data, the band model parameters are stored in an external file that is written in binary format; this allows for quicker access during the calculation. Each entry corresponds to a 1 cm^{-1} interval and contains a molecular parameter set. Since no data for molecules without lines in a given interval are stored, a parameter identifying the active species is included.

The first entry of a parameter set is the bin number, i. From the bin number, the midpoint of the interval is calculated

$$\nu_i = i \Delta\nu \quad , \quad (10)$$

and all lines whose centers fall in the half-opened interval ($\nu_i - \Delta\nu/2$, $\nu_i + \Delta\nu/2$) contribute to bin i.

The molecular parameter set is identified by the parameter m. The HITRAN database⁽²⁾ convention is used for this labeling

m	1	2	3	4	5	6	7	8	9	10	11	12
molecule	H ₂ O	CO ₂	O ₃	N ₂ O	CO	CH ₄	O ₂	NO	SO ₂	NO ₂	NH ₃	HNO ₃

The next entries in the parameter set are the molecular absorption coefficients (S/d) (cm⁻¹ amagats⁻¹) calculated at the five reference temperatures. These entries are followed by the STP Lorentz half width, γ_c^0 , multiplied by 10⁴ and stored as an integer. Line spacing parameters (1/d) for the five reference temperatures complete the line center parameter sets.

For line tails, each line contains data on one or two molecules. These line tail parameter sets use the same format as the line center parameter sets. Again, the first entry is the bin number i and the second entry is the molecule designation m. To recognize that these parameter sets denote line tail contributions, their molecule labels are offset by 12

m	13	14	15	16	17	18	19	20	21	22	23	24
molecule	H ₂ O	CO ₂	O ₃	N ₂ O	CO	CH ₄	O ₂	NO	SO ₂	NO ₂	NH ₃	HNO ₃

The continuum parameters, C, are stored in place of the (S/d). Unless all tail contributions have been defined for frequency bin i, the molecular designation and continuum parameters for a second molecule follow the first on the same parameter set.

A sample of the formatted data for frequency bins 2294 and 2295 is shown below:

2294	1	2.561E-07	9.816E-07	3.157E-06	8.694E-06	2.083E-05	592	1.814E+00	2.645E+00	3.273E+00	3.359E+00	3.182E+00
2294	2	1.384E+00	1.436E+00	1.598E+00	1.904E+00	2.377E+00	730	1.138E+00	1.775E+00	1.837E+00	2.486E+00	3.021E+00
2294	4	1.961E-03	2.842E-03	3.769E-03	4.681E-03	5.540E-03	757	2.227E+00	3.05E+00	2.517E+00	2.627E+00	2.720E+00
2294	13	1.681E-08	6.871E-08	2.090E-07	5.126E-07	1.071E-06	14	8.325E-02	7.507E-02	7.245E-02	7.535E-02	8.356E-02
2294	15	5.052E-09	5.037E-09	4.896E-09	4.678E-09	4.416E-09	16	3.339E-04	4.363E-04	5.346E-04	5.230E-04	6.978E-04
2294	18	3.393E-06	3.294E-06	3.529E-06	4.055E-06	4.816E-06	0	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
2295	2	3.195E-02	7.865E-02	1.678E-01	3.166E-01	5.403E-01	688	2.986E+00	2.537E+00	2.305E+00	2.217E+00	2.211E+00
2295	4	2.653E-05	3.804E-03	5.003E-03	6.174E-03	7.261E-03	766	2.729E+00	2.966E+00	3.161E+00	3.320E+00	3.449E+00
2295	5	1.511E-06	1.603E-06	1.659E-06	1.687E-06	1.691E-06	725	1.824E+00	1.898E+00	1.946E+00	1.975E+00	1.991E+00
2295	13	2.796E-08	1.118E-07	3.432E-07	8.628E-07	1.860E-06	14	1.309E-01	1.257E-01	1.302E-01	1.444E-01	1.675E-01
2295	16	3.903E-04	4.882E-04	5.769E-04	6.524E-04	7.129E-04	18	2.271E-06	3.374E-06	6.420E-06	9.811E-06	1.393E-05

In bin 2294, there are H₂O, CO₂ and N₂O line center parameter sets and tail data for H₂O, CO₂, O₃, N₂O and CH₄. In bin 2295, there is no line center data for H₂O, but lines do exist for CH₄. Also, bin 2295 does not contain any O₃ continuum data.

4. BAND MODEL TRANSMITTANCE FORMULATION

4.1 Line Center Transmittance

The band model transmittance formulation^(3,4) developed for the 5 cm^{-1} option to LOWTRAN 5⁽⁵⁾ has been used to create a moderate resolution option for LOWTRAN 7.⁽¹⁾ The expression used to calculate molecular transmittance is based on a statistical model for a finite number of lines within a spectral interval, and is given by

$$\tau = (1 - \langle W_{sg} \rangle / \Delta\nu)^{\langle n \rangle} , \quad (11)$$

where τ is the transmittance, $\langle W_{sg} \rangle$ is the Voigt single line equivalent width for the line strength distribution in a spectral interval, and $\langle n \rangle$ is the path averaged effective number of lines in the bin

$$\langle n \rangle = \Delta\nu \langle 1/d \rangle . \quad (12)$$

$\langle 1/d \rangle$ is the path averaged line spacing.

For large $\langle n \rangle$ [(S/d) and $\Delta\nu$ fixed], the transmittance simplifies to the more recognizable exponential form, Beer's Law, given by

$$\tau \rightarrow \exp(-\langle W_{sg} \rangle \langle 1/d \rangle) . \quad (13)$$

For the relatively low temperatures encountered in the earth's atmosphere, the number of lines in a bin from a single molecular species is usually small so that the power law transmittance formulation is preferred.

There are many approximations available for calculating the equivalent width of a Voigt line shape; different ones are valid for different regimes, Doppler or collision broadening, weak line or strong line, etc. However, no single approximation is adequate for the range of pressures and optical path lengths encountered in atmospheric transmission calculations. Rather than incorporating different approximations, we directly evaluate the exact expression for the equivalent width of a single line in a finite spectral interval; $\langle W_{sg} \rangle$ is given by

$$\langle W_{SA} \rangle = \frac{\Delta\nu}{X_m} \int_0^{X_m} 1 - \exp \{-[Su/d] \sqrt{\ln 2/\pi} F(X, Y)/\langle \gamma_d/d \rangle\} dX , \quad (14)$$

$$F(X, Y) = \frac{Y}{\pi} \int_{-\infty}^{\infty} \frac{\exp(-T^2)}{Y^2 + (X-T)^2} dT , \quad (15)$$

$$X_m = \frac{1}{2} \sqrt{\ln 2} \langle n \rangle / \langle \gamma_d/d \rangle , \quad (16)$$

$$Y = \sqrt{\ln 2} \langle \gamma_c/d \rangle / \langle \gamma_d/d \rangle , \quad (17)$$

where $F(X, Y)$ is the Voigt line shape function, $[Su/d]$ is the total optical depth, and $\langle \gamma_d/d \rangle$ and $\langle \gamma_c/d \rangle$ are the path averaged Doppler and collision broadened line shape band model parameters, respectively. To accurately calculate $\langle W_{SA} \rangle$, we separate its contributions as shown:

$$\langle W_{SA} \rangle = \langle W_{SA}^0 \rangle - \langle W_{SA}^1 \rangle , \quad (18)$$

$$\langle W_{SA}^0 \rangle = \frac{\Delta\nu}{X_m} \int_0^{\infty} 1 - \exp \{-[Su/d] \sqrt{\ln 2/\pi} F(X, Y)/\langle \gamma_d/d \rangle\} dX , \quad (19)$$

$$\langle W_{SA}^1 \rangle = \frac{\Delta\nu}{X_m} \int_{X_m}^{\infty} 1 - \exp \{-[Su/d] \sqrt{\ln 2/\pi} F(X, Y)/\langle \gamma_d/d \rangle\} dX , \quad (20)$$

The tail contribution, $\langle W_{SA}^1 \rangle$ can easily be evaluated in terms of the error function since $X_m \gg Y$ for cases calculated with MODTRAN:

$$\langle W_{SA}^1 \rangle \approx \exp(-z^2) + \sqrt{\pi} z \operatorname{erf}(z) - 1 , \quad (21)$$

$$z = \frac{2}{\langle n \rangle} \sqrt{[Su/d] \langle \gamma_c/d \rangle / \pi} . \quad (22)$$

To determine $\langle W_{SA}^0 \rangle$, an interpolation between the Lorentz and Doppler limits is used. Based on an interpolation formula developed by Ludwig,

et. al. [Equations (5-25) and (5-26)],⁽⁶⁾ the Lorentz and Doppler equivalent widths are given by

$$L = \frac{4}{4 + [Su/d]/\langle\gamma_c/d\rangle} \quad , \quad (23)$$

$$D = \frac{2}{\ln 2} \frac{\langle\gamma_d/d\rangle^2}{[Su/d]^2} \ln\left(1 + \frac{\ln 2}{2} \frac{[Su/d]^2}{\langle\gamma_d/d\rangle^2}\right) \quad , \quad (24)$$

$\langle w_{sl}^0 \rangle$ is determined from the following interpolation formula which is a more numerically stable form of their formula:

$$\langle w_{sl}^0 \rangle^2 = \frac{[Su/d]^2}{\langle 1/d \rangle^2} \left(1 - \frac{(1-L)(1-D)}{\sqrt{1-LD(2-L)(2-D)}}\right) \quad . \quad (25)$$

Figure 3 shows a comparison of Equation (25) to exact calculations for the equivalent width of a single, isolated spectral line with a Voigt lineshape. The lowest curve is the pure Doppler limit and the highest curve is the Lorentz limit. The exact values are taken from Penner.⁽¹⁵⁾ The predictions of Equation (25) are shown as solid lines for the same values of the parameter Y, Equation (17). The overall agreement between the two families of curves illustrates the quality of the interpolation formula.

4.1.1 Curtis-Godson Approximation

Path averages are calculated with the Curtis-Godson approximation.⁽⁶⁻⁸⁾ This approximation replaces an inhomogeneous path with a homogeneous one by using average values for the various band model parameters. The Curtis-Godson approximation is very good for paths where the temperature and concentration gradients are not particularly steep. This is the case for atmospheric paths where the temperature variations for

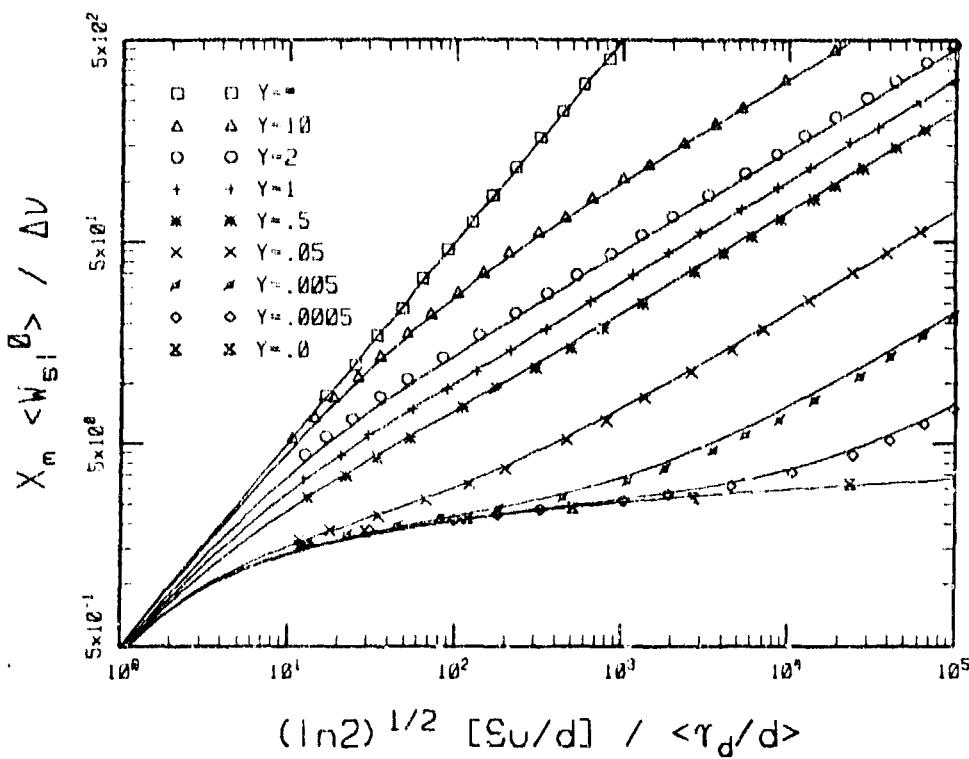


Figure 3. Curves of Growth for Spectral Lines with Combined Doppler and Lorentz Line Broadening. The Exact Calculations (15) are Presented as Individual Values. The NASA Formula, (6) Equation (25), is Shown as Solid Lines. The Values of Y From Bottom to Top are: 0, 0.0005, 0.005, 0.05, 0.5, 1.0, 2, 10, and ∞ .

arbitrary paths fall within the range of 200 to 300 K. The total optical depth is a sum over contributions from the individual layers and is given by

$$[Su/d] = \sum_k (S/d)_k (\Delta u)_k , \quad (26)$$

where $(\Delta u)_k$ is 'the' incremental absorber amount from layer k and $(S/d)_k$ is the absorption coefficient band model parameter at the temperature of the layer k . Note, frequency and species indices are implicitly assumed for this and subsequent equations.

The optical depth is used as the weighting function in calculating the path averages

$$\langle 1/d \rangle = \frac{1}{[Su/d]} \sum_k (1/d)_k (S/d)_k (\Delta u)_k , \quad (27)$$

$$\langle \gamma_c/d \rangle = \frac{1}{[Su/d]} \sum_k (\gamma_c)_k (1/d)_k (S/d)_k (\Delta u)_k , \quad (28)$$

$$\langle \gamma_d/d \rangle = \frac{1}{[Su/d]} \sum_k (\gamma_d)_k (1/d)_k (S/d)_k (\Delta u)_k . \quad (29)$$

The band model parameters were defined in the previous section, and $(\gamma_d)_k$ is the usual Doppler width (cm^{-1})

$$(\gamma_d)_k = \frac{v_i}{c} \sqrt{2(\ln 2) N k T / M} , \quad (30)$$

where M is equal to the molecular mass (g/mole) of the molecule and N is Avogadro's number.

4.2 Line Wing Absorption

The power law transmittance, Equation (11), takes into account only lines which originate within a given spectral interval, and, for these lines, only that fraction of the line profile which falls within the interval is included in the computation of the equivalent width. This approximation is reasonable in the strongly absorbing region of a band; however, because the absorptivity is expressed in terms of the local line strength distribution, it becomes a poor approximation in regions where the tail contributions from nearby lines dominate the contributions from weak or nonexistent lines within a given interval (bin). This typically occurs in the center and far wings of a band (i.e., past the band head), and also in spectral intervals containing no lines which are in the vicinity of strong lines. For these situations, the local absorption is dominated by the accumulated tails of the stronger lines located outside the interval. The effect of line wing absorption is included in the transmittance by adjoining an exponential term

$$\tau = (1 - \langle W_{B\Lambda} \rangle / \Delta\nu)^{\langle n \rangle} e^{-[Cu]} \quad , \quad (31)$$

where $[Cu]$ is the total continuum optical depth

$$[Cu] = \sum_k (C)_k (\Delta u)_k \quad . \quad (32)$$

The layer subscript k on C labels both the pressure [Equation (9)] and temperature (interpolated) dependencies.

5. INTEGRATION INTO LOWTRAN 7

Integration of the MODTRAN subroutines into LOWTRAN 7 was accomplished with minimal changes to the original code. The interface between the regular LOWTRAN 7 and the MODTRAN option is made through calls to two subroutines in the LOWTRAN 7 subroutine TRANS and one call in subroutine MSRAD. In TRANS, a single call to subroutine BMDATA reads the first necessary wavenumber block of band model parameters and calculates wavenumber independent quantities. For each wavenumber, calls to subroutine BMOD are made once for initialization and then additionally in the loop over atmospheric layers that calculates the molecular transmittance. In MSRAD, the call to FLXADD is replaced by a call to BMFLUX for the moderate-resolution option.

5.1 MODTRAN Subroutines

The MODTRAN subroutines are described in this section. In total, these six subroutines contain about 850 lines of code.

5.1.1 Subroutine BMDATA

Subroutine BMDATA is called once each calculation by subroutine TRANS. This subroutine opens the binary band model tape, makes the initial band model tape reads, and calculates wavenumber-independent quantities for subsequent use by subroutine BMOD.

After opening the band model tape, BMDATA reads the header information, advances the tape to the wavenumber block containing the initial frequency, IV1, and reads that block of data into common /BMDCOM/. If the requested spectral interval is totally outside of the band model tape range, the program simply performs a standard LOWTRAN 7 calculation.

For each atmospheric layer, wavenumber independent quantities are calculated in BMDATA and stored in the appropriate arrays for later use in BMOD. The quantities stored are $\sqrt{T/T_0}$ in arrays WT and WTS, and temperature interpolation indices in arrays JJ, FF, JJS and FFS. Arrays affixed with the letter 'S' define parameters for the solar paths.

5.1.2 Subroutine BMOD

Subroutine BMOD is the primary focus of the moderate resolution subroutines. In BMOD, the Curtis-Godson sums are calculated (Subsection 4.1.1), subroutine BMTRAN is called, and the continuum contributions due to tails of lines originating outside the 1 cm^{-1} interval are determined. An initialization call is made every wavenumber from subroutine TRANS, and subsequent calls are made for each layer to calculate the transmittance. On the first call, BMOD retrieves band model data through calls to BMLOAD, initializes the Curtis-Godson sums, determines the frequency dependent Doppler line widths, Equation (30), and reads the next frequency block of band model parameters if necessary (IP is the counting variable). On subsequent calls, the Curtis-Godson approximation is used to calculate optical depth (SDSUM), line density (ODSUM), Lorentz half width (COLSUM) and Doppler half width (DOPSUM). The contributions from tails of lines are also calculated within the layer loop. Since these tails have a smooth spectral structure, they form a continuum component, and the simple exponential form, Equation (31), is used to calculate the transmittance. These tail contributions and the molecular components from BMTRAN are combined (multiplied together) and stored in the matrix TX for subsequent use by subroutine TRANS.

The calls made by TRANS to BMOD for calculating the transmittance is embedded in a loop over atmospheric layers. When only the transmittance is calculated, the DO-loop in TRANS consists of one pass. When atmospheric radiation is calculated, the TRANS loop is over all layers, because the radiation depends on the incremental change in transmittance for each layer. The Curtis-Godson approximation for the statistical band model requires the sum over layers for transmittance calculations. In keeping with the philosophy of minimizing changes to the basic LOWTRAN 7 program, this layer loop is done in BMOD for transmittance-only calculations and in TRANS for radiation calculations. Thus, the layer loop in BMOD consists of just one pass when TRANS is looping over all layers and vice-versa. Subroutine BMOD determines whether the loop in TRANS is over one layer or all layers and then adjusts its own loop variable accordingly.

5.1.3 Subroutine BMLOAD

Subroutine BMLOAD (called by BMOD) loads band model data for a single parameter set into the matrices SD, OD and ALFO.

5.1.4 Subroutine BMTRAN

BMTRAN is called by subroutine BMOD to calculate finite bin molecular transmittances. The curve-of-growth used in the statistical band model is based on the equivalent width of a single average line in a 1 cm^{-1} interval. Band model parameters are calculated in BMOD for an equivalent homogeneous path, using the Curtis-Godson approximation.

As discussed in Subsection 4.1, the Voigt line shape is integrated over the interval. When the optical depth is less than .001, the weak line limit is used. Otherwise, the Voigt line shape is calculated from Equations (18) - (25).

5.1.5 Subroutine BMERFU

BMERFU is called by BMTRAN to calculate the finite bin width correction to the Voigt integral, Equations (21) and (22). For small non-negative z , the error function is calculated from the rational approximation given by Abramowitz and Stegun, Equation (7.1.26).⁽¹⁶⁾ For large z , the error function is determined as a continued fraction derived from the asymptotic expansion, Equation (7.1.23) of Reference 16.

5.1.6 Subroutine BMFLUX

BMFLUX is the moderate resolution version of the LOWTRAN-7 subroutine FLXADD. Called by MSRAD, BMFLUX is used to sum optical thicknesses, to compute the diffuse thermal and solar flux contributions from a two-stream approximation, and to combine these fluxes in an adding routine which determines total upward and downward fluxes for each layer. The k -distribution method is not used in this fast version of FLXADD. Since the spectral intervals in the MODTRAN calculations are only 1 cm^{-1} , it

treats these transmittances as monochromatic for the multiple-scattering fluxes. Thus, the molecular optical depth of a layer is calculated in MSRAD as a logarithm of molecular transmittances.

5.2 Modifications to LOWTRAN 7

Modifications to LOWTRAN 7 have been kept to a minimum. As mentioned in Section 2, the switch MODTRN has been added to /CARD1/. Only if MODTRN is .TRUE. are any of these changes activated.

Most of the routines from LOWTRAN 7 remain unchanged. A number of routines have been modified only in that the blank common along with the labeled commons /CARD1/, /CARD4/, /SOLS/ and /TRAN/ have been changed. These routines are ABCDTA, AEREEXT, AERNSM, CIRR18, CIRRUS, CLDPRF, DESATT, EQULWC, EXABIN, FLXADD, LAYVSA, PHASEF, RDEXA, RDNSM, RFPATH, SSRAD and VSANSM.

A number of routines have undergone minor modifications. Routines GEO and SSGEO were altered in order to make the following changes/additions:

- The matrices WPATH (WPATHS) and WPMS (WPMSS) have been combined into the single matrix WPATH (WPATHS),
- Layer pressures and temperatures are stored for use by the band model routines, and
- Curtis-Godson averaged pressures and temperatures are determined for solar paths.

STDMDL calculates actual rather than scaled molecular column densities when MODTRN is .TRUE.. Finally, routine MSRAD computes molecular optical thicknesses and calls routine BMFLUX.

Significant changes were made to the MAIN. It has been split into two routines. The new MAIN consists of almost 1000 lines of introductory comments and a single call to the new subroutine DRIVER. DRIVER is the driver for MODTRAN and it contains all the executable statements from LOWTRAN 7's MAIN. In addition, it defines a pointer array called KPOINT that maps the HITRAN molecular labels (1-12) into the LOWTRAN 7 labels. Also, DRIVER checks the spectral inputs. For moderate resolution, the

variables IV1, IV2 and IDV need not be multiples of 5, and the additional variable IFWHM must be read.

Considerable modifications were required for TRANS. When MODTRN is .TRUE., TRANS

- sets the internal frequency step size to 1 cm^{-1} ,
- calls the MODTRAN subroutines to calculate molecular transmittance,
- interpolates transmittances calculated at 5 cm^{-1} intervals for the aerosols and molecular continua, and
- employs a discretized triangular slit function with FWHM set to IFWHM to automatically degrade the 1 cm^{-1} bin results to the requested spectral resolution.

In Subsections 5.1.1 and 5.1.2, the calls to the MODTRAN subroutines were discussed. Note that the discretized triangular slit function when IFWHM is set to 1 cm^{-1} is a 1 cm^{-1} rectangular slit function, as shown in Figure 4. The figure also demonstrates that, when the printing step size parameter IDV (=2 here) is larger than IFWHM, the frequency range is under sampled.

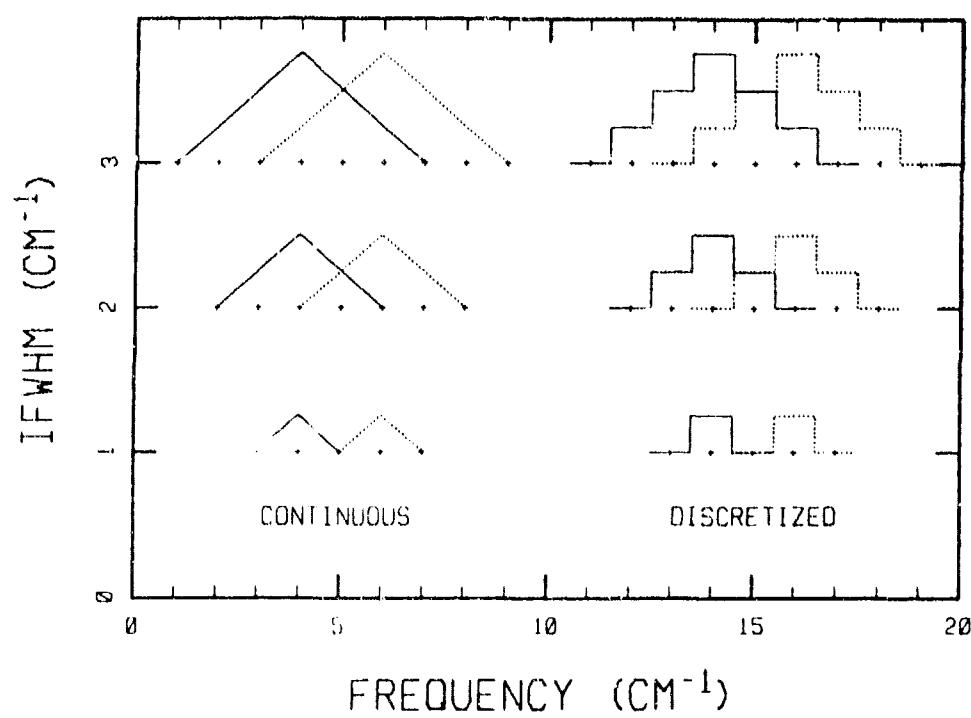


Figure 4. Comparison of Continuous and Discretized Triangular Slit Functions. FASCOD2 Uses the Weighting from the Continuous Function, but MODTRAN Uses the Discretized Approximation. For this Example, IDV = 2 and the Curves are Shown for IFWHM = 1, 2, and 3.

6. VALIDATION

Tests were performed to ensure the band model parameters were generated correctly, and MODTRAN transmittances and radiances were validated by comparing to FASCOD2 line-by-line calculations. A few comparisons follow.

6.1 Band Model Parameters

The 1 cm^{-1} band model parameters were checked against the moderate resolution LOWTRAN 5^(3,4) 5 cm^{-1} values. A straightforward degradation of the newer higher resolution parameters was performed. In Figure 5,

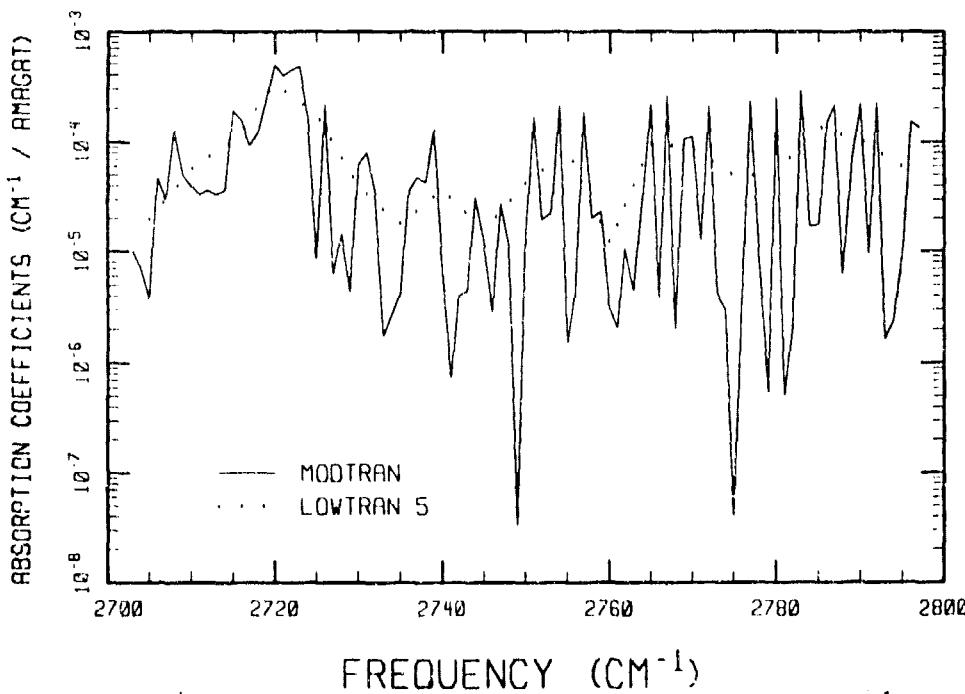


Figure 5. Comparison of Band Model LOWTRAN 5 (Dotted Curve) and MODTRAN (Solid Curve) Molecular Absorption Coefficients for Water Vapor at 300 K.

absorption coefficients from both sets of parameters before degradation are plotted. When degraded, the 1 cm^{-1} parameters are indistinguishable from the curve with the LOWTRAN 5 band model parameters.

6.2 Comparison with FASCOD2

In Figure 6, MODTRAN and FASCOD2 transmittances are compared for a low altitude slant path through the US Standard Atmosphere in the spectral region $2160 - 2260 \text{ cm}^{-1}$. The curves were generated with a 2 cm^{-1} triangular slit function (FWHM). The absorption in this region is primarily due to the N_2O band centered at 2224 cm^{-1} and the P branch of the $4.3 \mu\text{m}$ CO_2 band. Although the agreement is very good, discrepancies do exist. The dip at 2210 cm^{-1} stands out. The N_2O lines in this region are spaced about 0.8 to 0.9 cm^{-1} apart, and therefore most 1 cm^{-1} bins contain just one line. The bin at 2210 cm^{-1} is an exception containing two lines,

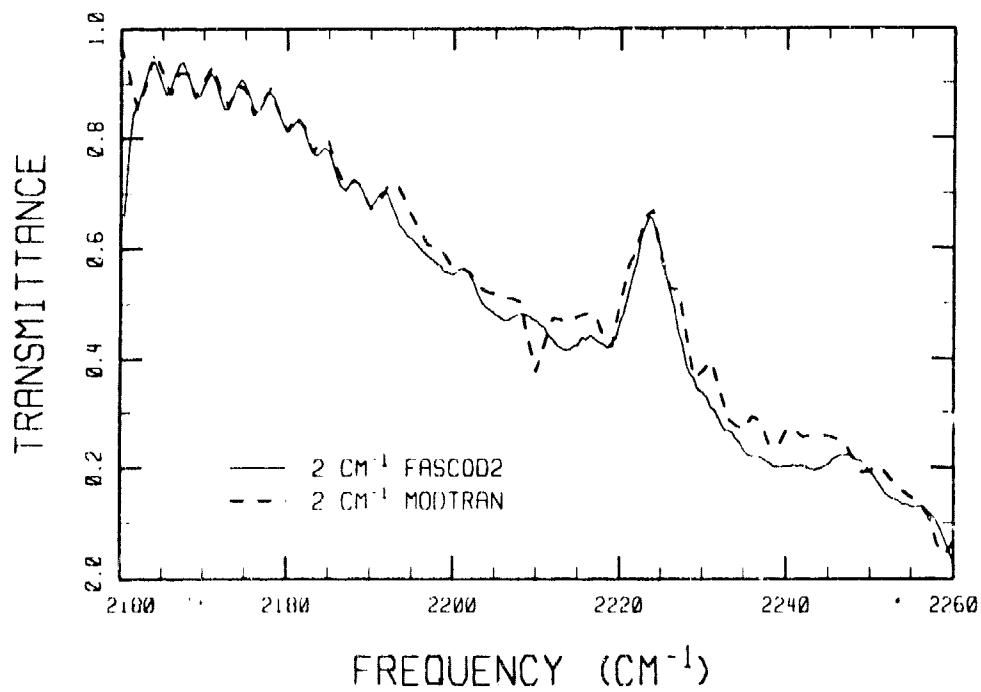


Figure 6. Comparison of a FASCOD2 and a MODTRAN Calculation. N_2O and CO_2 are the Primary Absorbers.

resulting in the dip. Similar analysis can be applied to other discrepancies and implies that better agreement results with some further degradation of the spectral resolution.

Since the band model parameters were generated down to 0 cm^{-1} , MODTRAN can be used to perform molecular absorption calculations in the microwave region. Results for a 0.1 km sea level path through the US Standard Atmosphere are compared to FASCOD2 in Figure 7. The dominant absorber throughout this region is water. The calculations compare well.

As discussed in Section 2, the LOWTRAN 7 and MODTRAN implementations of the multiple scattering routines are different. LOWTRAN uses the k-distribution method to approximate the multiple scattering contribution to each 5 cm^{-1} interval as the sum of three monochromatic calculations. The basic idea is to partition the range of absorption coefficients occurring in the 5 cm^{-1} interval into three representative values, each weighted according to the size of the sub-interval it represents. Since the intervals in MODTRAN are only 1 cm^{-1} wide, the partitioning into

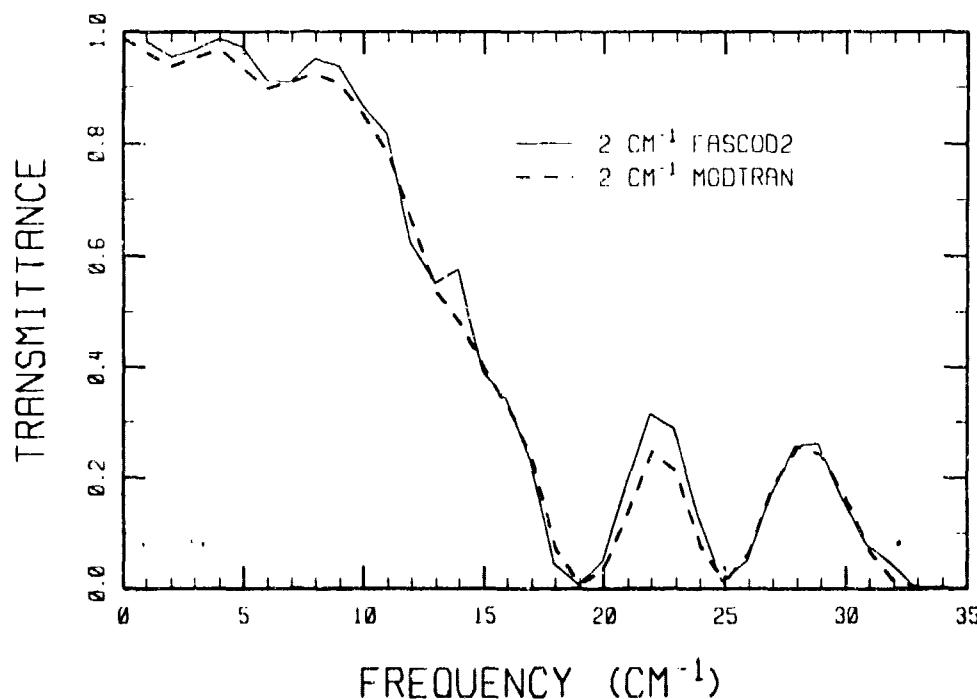


Figure 7. Comparison of a FASCOD2 and a MODTRAN Calculation in the Microwave Region. The Calculation was Performed Using a 0.1 km Horizontal Path at 0 km Altitude and with No Haze.

sub-intervals has been eliminated, and a single average absorption coefficient is used for each bin.

Figure 8 shows a comparison of a LOWTRAN 7 multiple scattering calculation (dotted line) to a MODTRAN multiple scattering calculation (solid line) from $.6$ to $.7 \mu\text{m}$, each at 20 cm^{-1} resolution and with a step size of 5 cm^{-1} . The atmospheric profile is the U. S. Standard, and the calculation is performed using the rural extinction atmospheric haze model with a ground visibility of 5 km . The observer is at an altitude of 20 km looking straight up, and the sun is 60° from zenith. For this calculation, thermal radiance is negligible and the contribution of single scattering (dashed line) is only about 15% of the total signal; the radiance is dominated by multiple scattering. Agreement between the two calculations is excellent, the main difference being the increased spectral structure in the MODTRAN calculation.

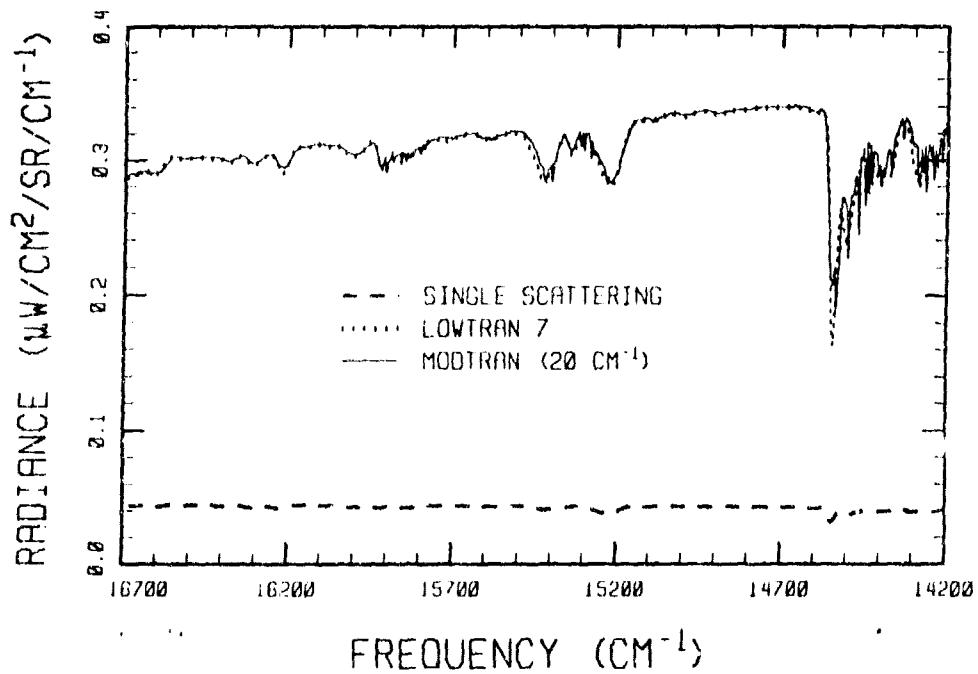


Figure 8. Comparison of Radiances from LOWTRAN 7 and MODTRAN ($\text{FWHM}=20\text{cm}^{-1}$), Both with Multiple Scattering. Visibility is 5 km and the Sun is 60° from Zenith. The Observer is at 20 km Altitude Looking Straight up.

LOWTRAN 7 and MODTRAN also differ in their approaches to handling molecular transmittance. Since the LOWTRAN model has been optimized for 296 K, sea level paths, LOWTRAN should not be used for atmospheric paths completely above 30 km. MODTRAN, on the other hand, uses a Voigt lineshape, which is applicable at higher altitudes. Figures 9-11 demonstrate MODTRAN's high altitude capabilities. First, Figure 9 shows that LOWTRAN 7 and MODTRAN do indeed predict vastly different radiances at higher altitudes. Radiation levels from H_2O rotations along a 60 km limb path are shown. The LOWTRAN spectral radiances are much too low at these altitudes. To demonstrate that MODTRAN calculations are correct, validations have been performed against SHARC,^(17,18) the Strategic High Altitude Radiation Code. SHARC performs NLTE (non-local thermodynamic equilibrium) calculations from 60 to 300 km altitude. However, at 60 km, vibration state populations are essentially LTE and H_2O rotations are always treated as LTE in SHARC, so comparisons between MODTRAN and SHARC should produce similar results. With a 60 km limb path, the two codes predict similar spectral radiances for H_2O rotations (Figure 10) and for the 15 μm CO_2 band (Figure 11), which is mostly LTE. The SHARC calculations were done at a spectral resolution of 0.5 cm^{-1} and degraded to 1 cm^{-1} (FWHM).

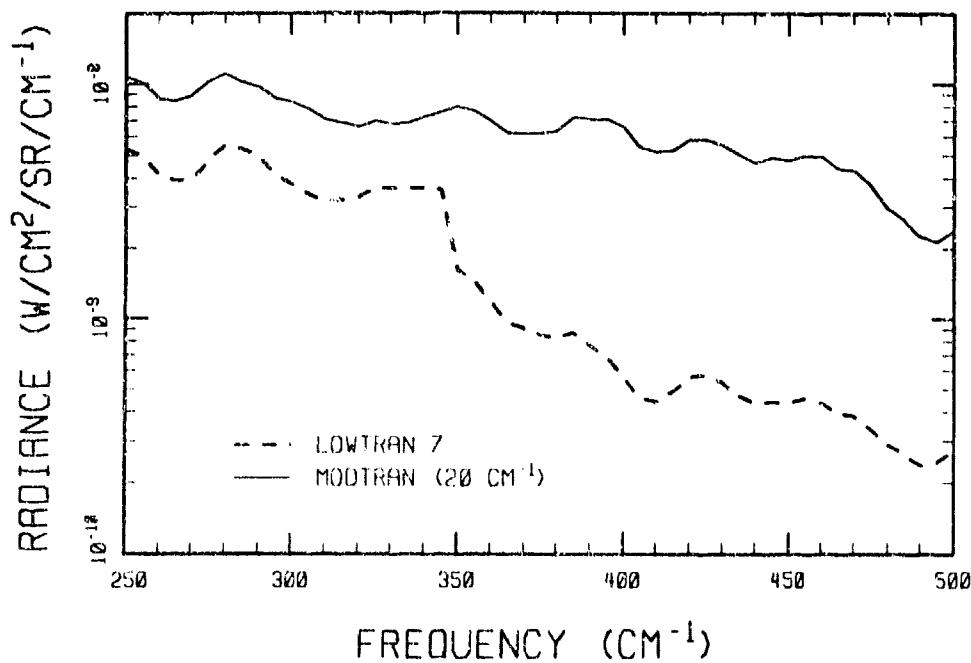


Figure 9. LOWTRAN 7 and MODTRAN Predictions for Radiation from the H₂O Rotational Band for a 60 km Limb Path. At These Altitudes, LOWTRAN Underpredicts the Radiance.

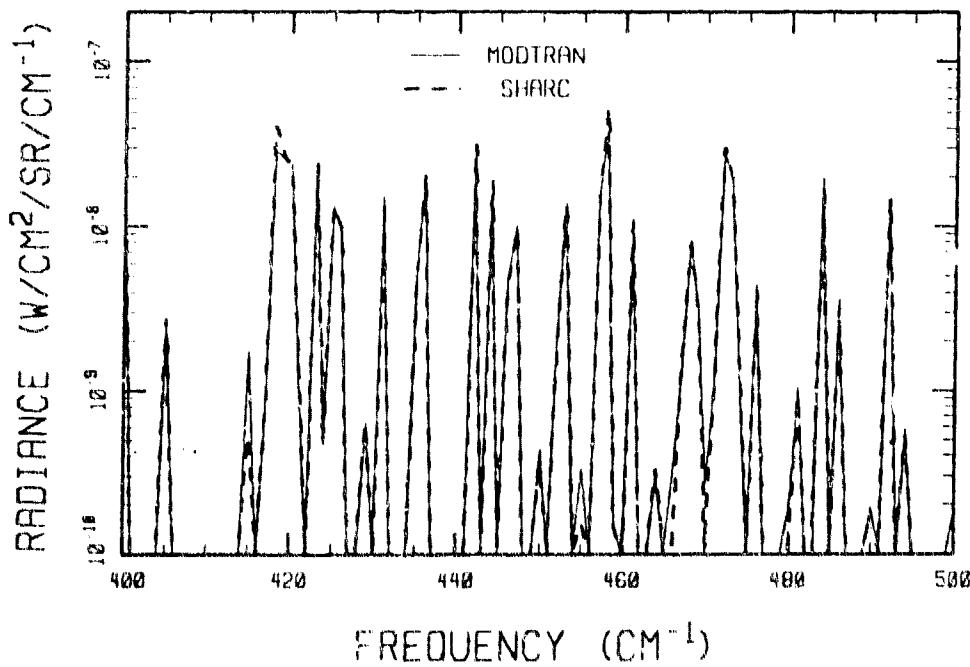


Figure 10. MODTRAN and SHARC Predictions of H₂O Rotations for 60 km Limb.

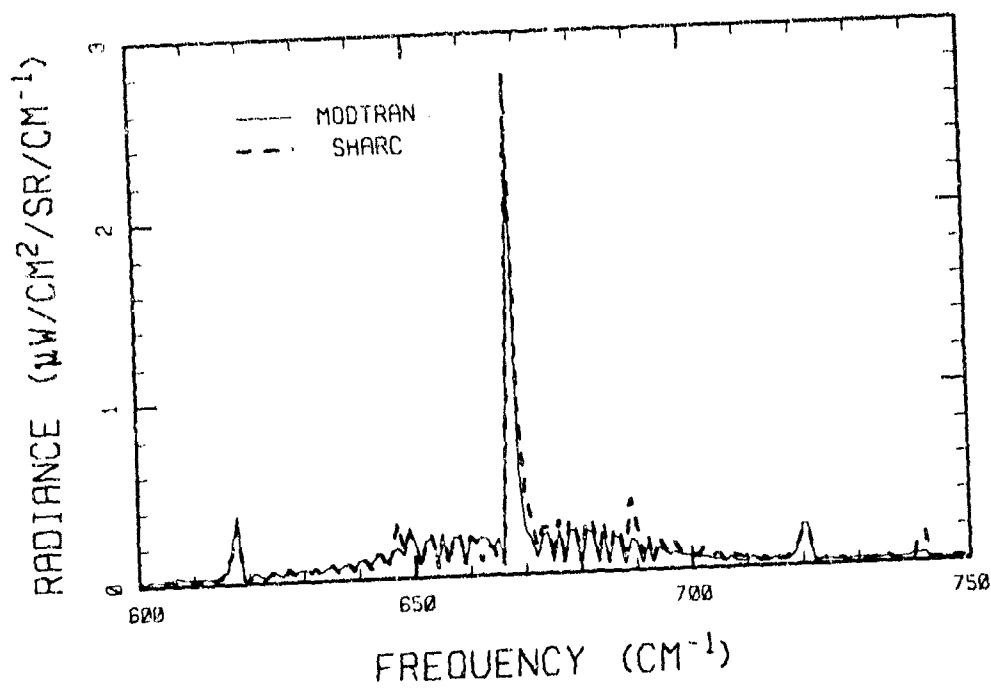


Figure 11. MODTRAN and SHARC Predictions of the 15 μm CO₂ Band for 60 km Limb.

7. CONCLUSIONS

A radiative transfer model with a spectral resolution of 2 cm^{-1} (FWHM) has been developed based on the LOWTRAN 7 model. The new code has been given the name MODTRAN (Moderate resolution LOWTRAN). Initial validation studies, based on comparisons to FASCOD2, indicate no significant discrepancies at 2 cm^{-1} resolution, FWHM. MODTRAN can be used to calculate atmospheric radiance at upper altitudes, specifically for any path in which the LTE (local thermodynamic equilibrium) approximation is valid. Molecular absorption is modeled as a function of both temperature and pressure for twelve molecular species - water vapor, carbon dioxide, ozone, nitrous oxide, carbon monoxide, methane, oxygen, nitric oxide, sulfur dioxide, nitrogen dioxide, ammonia and nitric acid. MODTRAN also has a multiple scattering option which enables the code to calculate both thermal and solar multiple scattering contributions. A final version of the code has been delivered to the Geophysics Laboratory.

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APPENDIX

In MODTRAN, the molecular transmittance, τ , from lines originating within a spectral bin, $\Delta\nu$, is determined from an expression of the form

$$\tau = \left(\frac{2}{\Delta\nu} \int_0^{\Delta\nu/2} e^{-Sb(v) dv} \right)^n \quad (A-1)$$

where $b(v)$ is a line shape function, u is the absorber amount, and S and n are functions of the absorption coefficient (S/d) and line density (l/d) band model parameters

$$S = \frac{(S/d)}{(l/d)} \quad , \quad (A-2)$$

$$n = (l/d) \Delta\nu \quad , \quad (A-3)$$

Equation (A-1) compare to Equations (11) and (14).

A standard method for determining band model parameters was laid out by Goody. (19) The weak and strong line limits of a two parameter transmittance expression are determined. These results are equated to the weak and strong line limits of the Ladenburg-Reiche function, and the resulting equations are solved for the unknown parameters. When Goody applied his approach to two trial transmittance formulas, both gave expressions for the band model parameters of the form

$$(S/d) = \frac{1}{\Delta\nu} \sum_{i=1}^N s_i \quad , \quad (A-4)$$

$$(l/d) \approx \frac{1}{\Delta\nu} \left(\sum_{i=1}^N \sqrt{s_i} \right)^2 / \sum_{i=1}^N s_i \quad . \quad (A-5)$$

Here, N is the number of lines and S_i is the integrated line strength of line i (the line spacing formula assumes all N lines have the same half width).

It is worth noting that Goody's approach is not quite appropriate for the transmittance expression in MODTRAN. Equation (A-1) models the transmittance through a set of lines whose centers fall within a given finite spectral bin. The Ladenburg-Reiche function, on the other hand, models the total absorption due to those lines - not just their contribution within a finite spectral bin.

Instead of equating the weak and strong line limit of Equation (A-1) to the Ladenburg-Reiche function, we equate the weak and strong line limit of Equation (A-1) to Plass' expression⁽²⁰⁾ for the transmission due to lines whose centers are randomly distributed in a given spectral interval,

$$\left(\frac{2}{\Delta\nu} \int_0^{\Delta\nu/2} \exp[-\text{Sub}(\nu)] d\nu \right)^N \approx n_i \left(\frac{2}{\Delta\nu} \int_0^{\Delta\nu/2} \exp[-S_i \text{ub}(\nu)] d\nu \right)^N . \quad (\text{A-6})$$

Here, all N lines are assumed to have the same half width, but the line shape function is arbitrary.

If B_j is defined by the equation

$$B_j = \frac{2}{\Delta\nu} \int_0^{\Delta\nu/2} [-b(\nu)]^j / j! d\nu , \quad (\text{A-7})$$

then, in the weak line limit, Equation (A-7) becomes

$$1 + u (B_1 n_i S_i) + u^2 \left[\frac{B_1^2}{2} (n_i S_i)^2 + (B_2 - \frac{B_1^2}{2}) n_i S_i^2 \right] + O(u^3) =$$

$$1 + u (B_1 \sum_{i=1}^N S_i) + u^2 \left[\frac{B_1^2}{2} \left(\sum_{i=1}^N S_i \right)^2 + (B_2 - \frac{B_1^2}{2}) \sum_{i=1}^N S_i^2 \right] + O(u^3) . \quad (\text{A-8})$$

The first order equation in u reestablishes Equation (A-4)

$$n S = \sum_{i=1}^N S_i \quad . \quad (A-9)$$

To determine the strong line limit of Equation (A-6), we assume $b(v)$ to be a non-increasing bounded positive function on $[0, \infty)$. Consider a general integral of the form

$$I = \frac{2}{\Delta v} \int_0^{\Delta v/2} e^{-S u b(v)} dv \quad . \quad (A-10)$$

It follows that

$$0 < e^{-S u b(0)} < I < e^{-S u b(\Delta v/2)} < 1 \quad . \quad (A-11)$$

This inequality requires that I falls off exponentially with large u and that the exponent is linear in u . The exponential decay factor, C , is given by the limit as $u \rightarrow \infty$ of the negative logarithm of I divided by u

$$C = - \lim_{u \rightarrow \infty} [\ln(I)/u] \quad . \quad (A-12)$$

Applying L'hopital's rule, one obtains

$$C = S \langle b(v) \rangle \quad , \quad (A-13)$$

where

$$\langle b(v) \rangle = \lim_{u \rightarrow \infty} \frac{\int_0^{\Delta v/2} b(v) e^{-S u b(v)} dv}{\int_0^{\Delta v/2} e^{-S u b(v)} dv} \quad . \quad (A-14)$$

Note that this limit is independent of the value of S as long as $S > 0$.

Taking the logarithm of both sides of Equation (A-6), dividing by u , and equating the asymptotic limits, one obtains

$$n S \langle b(v) \rangle = \sum_{i=1}^N S_i \langle b(v) \rangle \quad . \quad (A-15)$$

Since $\langle b(\nu) \rangle$ is line independent, the surprising result is that Equation (A-9), the weak line limit, is also the strong line limit!

To determine n and S , we return to the weak line limit, Equation (A-8), and consider the equation obtained from the coefficient of the quadratic terms in u . This equation gives

$$n S^2 = \sum_{i=1}^N s_i^2 . \quad (A-16)$$

The resulting expressions for the band model parameters are

$$(S/d) = \frac{1}{\Delta\nu} \sum_{i=1}^N s_i , \quad (A-4)$$

$$(1/d) = \frac{1}{\Delta\nu} \left(\sum_{i=1}^N s_i \right)^2 / \sum_{i=1}^N s_i^2 . \quad (A-17)$$

(S/d) has the same form as before, but a smaller value for $(1/d)$ is obtained.